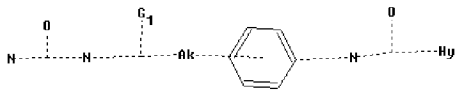
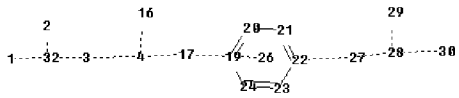
=>
Uploading C:\Program Files\Stnexp\Queries\10555286-elected-103.str





chain nodes :
1 2 3 4 5 6 7 16 17 27 28 29 30 32
ring nodes :
8 9 10 11 12 19 20 21 22 23 24
chain bonds :
1-32 2-32 3-4 3-32 4-16 4-17 5-6 5-7 22-27 27-28 28-29 28-30
ring bonds :
8-9 8-12 9-10 10-11 11-12 19-24 19-20 20-21 21-22 22-23 23-24
exact/norm bonds :
1-32 2-32 3-4 3-32 4-16 4-17 5-6 5-7 8-9 8-12 9-10 10-11 11-12 22-27
27-28 28-29 28-30
normalized bonds :
19-24 19-20 20-21 21-22 22-23 23-24
isolated ring systems :
containing 8 : 19 :

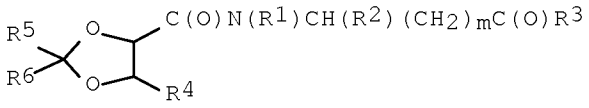
G1:[*1],[*2]

Connectivity :
17:2 E exact RC ring/chain
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:Atom 9:Atom
10:Atom
11:Atom 12:Atom 16:CLASS 17:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom
24:Atom
26:Atom 27:CLASS 28:CLASS 29:CLASS 30:Atom 32:CLASS
Generic attributes :
30:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : Exactly 1
Type of Ring System : Monocyclic

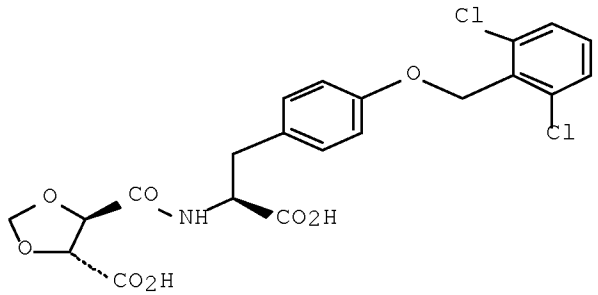
Element Count :
Node 30: Limited
C,C5
N,N1

L14 STRUCTURE UPLOADED

```
=> d his

L14             STRUCTURE UPLOADED
L16          55 S L14 SSS FULL

     FILE 'CAPLUS' ENTERED AT 16:50:48 ON 11 JUL 2008
L17           4 S L16

=> d l17 tot bib abs hitstr

L17  ANSWER 1 OF 4  CAPLUS  COPYRIGHT 2008 ACS on STN
AN   2005:260065  CAPLUS  Full-text
DN   142:316825
TI   Preparation of dioxolane derivatives as cell adhesion inhibitors with
     therapeutic uses
IN   Palle, Venkata P.; Sattigeri, Viswajanani J.; Salman, Mohammad; Soni,
     Ajay; Ray, Abhijit; Dastidar, Sunanda G.
PA   Ranbaxy Laboratories Limited, India
SO   PCT Int. Appl., 132 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.         DATE
     ---------------     ----   --------    --------------------    --------
PI   WO 2005026163        A1    20050324    WO 2004-IB3047          20040917
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
     EP 1668007          A1    20060614    EP 2004-769418          20040917
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
     IN 2006DN01690      A     20070323    IN 2006-DN1690          20060328
PRAI US 2003-503643P     P     20030917
     WO 2004-IB3047      W     20040917
OS   CASREACT 142:316825; MARPAT 142:316825
GI
```



I



II

AB The present invention relates to dioxolane derivs. (shown as I; variables defined below; e.g. (4R,5R)-5-[[(S)-1-carboxy-2-[4-(2,6-dichlorobenzyloxy)phenyl]ethyl]carbamoyl]-[1,3]dioxolane-4-carboxylic acid (shown as II)), their pharmaceutically acceptable salts, pharmaceutically acceptable solvates, enantiomers, diastereomers, polymorphs or N-oxides as cell adhesion inhibitors (no data). These compds. can be useful for inhibition and prevention of cell adhesion and cell adhesion-mediated pathologies, including inflammatory and autoimmune diseases such as bronchial asthma, rheumatoid arthritis, type I diabetes, multiple sclerosis, allograft rejection or psoriasis. This invention also relates to pharmacol. compns. containing the compds. of the present invention, and the methods of treating bronchial asthma, rheumatoid arthritis, multiple sclerosis, type I diabetes, psoriasis, allograft rejection, and other inflammatory and/or autoimmune disorders, using the compds. For I: m = 0-2; R1 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl, heteroarylalkyl, or heterocyclylalkyl; R2 = H, alkyl, alkenyl, alkynyl, cycloalkyl, carboxy, aryl, aralkyl, heteroaryl, heterocyclyl, heteroarylalkyl, or heterocyclylalkyl; R1 and R2 may together join to form a cyclic ring (3-8 membered), which may be optionally benzo-fused, containing 0-4 heteroatoms such as O, S, or N, wherein the rings may be substituted with ≥1 alkyl, alkenyl, alkynyl, (un)substituted amino, cycloalkyl, carboxy, alkoxy, aryloxy, halogen, aryl, aralkyl, heteroaryl, heterocyclyl, heteroarylalkyl or heterocyclylalkyl. R3 = NH2, NHOH, NHOR (R = alkyl, alkenyl, alkynyl, cycloalkyl or aralkyl), or ORm (Rm = H, alkyl, aralkyl, aryl, or metal ions (Na, K, Li, Ca or Mg)); R4 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl, heteroaryl, heterocyclyl, heteroarylalkyl, heterocyclylalkyl, -(CH2)1-4-OR' (R'= H, alkyl, alkenyl, alkynyl, aralkyl, aryl, heterocyclylalkyl, or heteroarylalkyl), -C(O)R3, -C(O)Rz (Rz is -NR7R8, R7 and R8 = H (provided that both R7 and R8 are not H, represented as amino), alkyl, alkenyl, alkynyl, aralkyl, cycloalkyl, hydroxyalkyl, aralkyloxy, aryl, heteroaryl, heterocyclyl, heteroarylalkyl, heterocyclylalkyl, SO2R9 (R9 = alkyl, alkenyl, alkynyl, cycloalkyl, aralkyl, aryl, heterocyclyl, heteroaryl, heteroarylalkyl, heterocyclylalkyl)). Or R7 and R5 may together join to form a cyclic ring (3-8 membered), which may be optionally benzo-fused, containing 0-4 heteroatoms such as O, S, or N, wherein the rings may be substituted with ≥1 of alkyl, alkenyl, alkynyl, (un)substituted amino, cycloalkyl, carboxy, alkoxy, hydroxy, oxo, aryloxy, aryl, halogen, aralkyl, heteroaryl, heterocyclyl, heteroarylalkyl, or heterocyclylalkyl; or (CH2)1-4NRxRy (Rx and Ry = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl, heteroaryl, heterocyclyl, heterocyclylalkyl, heteroarylalkyl, -YRu (Y is C(O), C(S) or SO2 and Ru is alkyl, alkenyl, alkynyl, aryl, aralkyl, heteroaryl, heterocyclyl,

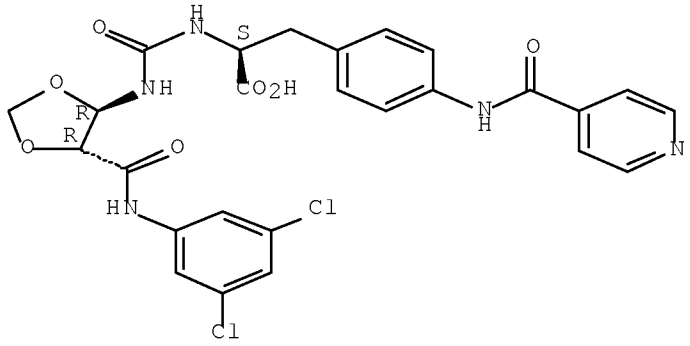
heterocyclylalkyl or heteroarylalkyl), -C(:T)NRu (T is O, S, -CH(NO2), -N(NO2) or -N(CN)) or -C(O)ORu); R5 and R6 = H, alkyl, cycloalkyl, heterocyclyl, heteroarylalkyl, heterocyclylalkyl, aryl, or aralkyl; or R5 and R6 may together join to form a cycloalkyl ring. Methods of preparation of I and intermediates are claimed and 14 example prepns. are included. For example, II was prepared in 4 steps starting from di-Et (4R,5R)-[1,3]dioxolane-4,5-dicarboxylate and involving intermediates (4R,5R)-[1,3]dioxolane-4,5-dicarboxylic acid monoethyl ester, (4R,5R)-5-[[(S)-1-(benzyloxycarbonyl)-2-(4-hydroxyphenyl)ethyl]carbamoyl]- [1,3]dioxolane-4-carboxylic acid Et ester, and (4R,5R)-5-[[(S)-1- (benzyloxycarbonyl)-2-[4-(2,6-dichlorobenzyloxy)phenyl]ethyl]carbamoyl]- [1,3]dioxolane-4-carboxylic acid Et ester.

IT 848210-00-4P, (S)-2-[[[(4R,5R)-5-(3,5-Dichlorophenylcarbamoyl)-[1,3]dioxolan-4-yl]carbamoyl]amino]-3-[4-[[(pyridin-4-yl)carbonyl]amino]phenyl]propionic acid
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of dioxolane derivs. as cell adhesion inhibitors with therapeutic uses)

RN 848210-00-4 CAPLUS

CN L-Phenylalanine, N-[[[(4R,5R)-5-[[(3,5-dichlorophenyl)amino]carbonyl]-1,3-dioxolan-4-yl]amino]carbonyl]-4-[(4-pyridinylcarbonyl)amino]- (CA INDEX NAME)

Absolute stereochemistry.

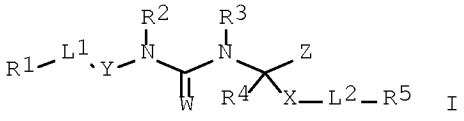


RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

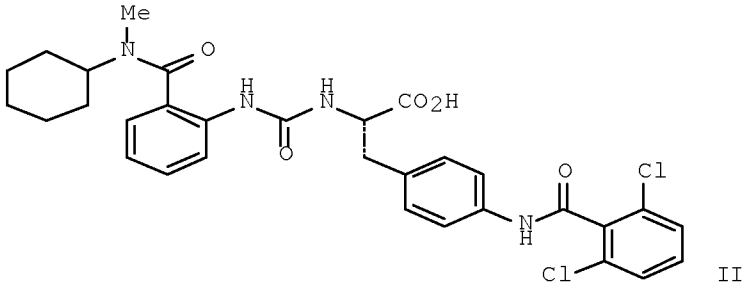
L17 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2002:555472 CAPLUS Full-text
DN 137:125085
TI Preparation of urea derivatives as integrin alpha 4 antagonists
IN Jimenez Mayorga, Juan Miguel; Bach Tana, Jordi; Ontoria Ontoria, Jesus Maria; Navarro Romero, Eloisa
PA Almirall Prodesfarma, S.A., Spain
SO PCT Int. Appl., 107 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI WO 2002057242 A2 20020725 WO 2002-EP331 20020115
WO 2002057242 A3 20031127
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
ES 2200617 A1 20040301 ES 2001-126 20010119
ES 2200617 B1 20050501
CA 2434939 A1 20020725 CA 2002-2434939 20020115
AU 2002228048 A1 20020730 AU 2002-228048 20020115
AU 2002228048 B2 20080313
EE 200300327 A 20031015 EE 2003-327 20020115
EP 1383750 A2 20040128 EP 2002-710010 20020115
EP 1383750 B1 20070926
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
HU 2003003722 A2 20040301 HU 2003-3722 20020115
HU 2003003722 A3 20051228
JP 2004517143 T 20040610 JP 2002-557923 20020115
BR 2002006588 A 20040622 BR 2002-6588 20020115
CN 1531425 A 20040922 CN 2002-806525 20020115
NZ 527031 A 20050930 NZ 2002-527031 20020115
RU 2296120 C2 20070327 RU 2003-125367 20020115
AT 374191 T 20071015 AT 2002-710010 20020115
ES 2291448 T3 20080301 ES 2002-710010 20020115
IN 2003DN01102 A 20070302 IN 2003-DN1102 20030715
MX 2003PA06363 A 20040420 MX 2003-PA6363 20030716
ZA 2003005535 A 20041018 ZA 2003-5535 20030717
NO 2003003269 A 20030919 NO 2003-3269 20030718
BG 108004 A 20040930 BG 2003-108004 20030718
HK 1058361 A1 20071207 HK 2004-101137 20040218
US 20040142982 A1 20040722 US 2004-466665 20040223
US 7253171 B2 20070807
US 20070238763 A1 20071011 US 2007-802165 20070521
PRAI ES 2001-126 A 20010119
WO 2002-EP331 W 20020115
US 2004-466665 A3 20040223
OS MARPAT 137:125085
GI



I



II

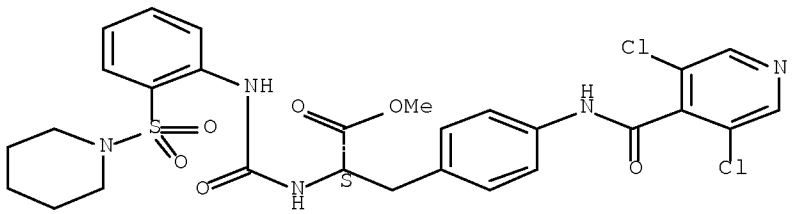
AB The title compds. [I; R1 = alkyl, alkenyl, cycloalkyl, etc.; R2 = H, alkyl, alkylaryl, etc.; R3, R4 = H, alkyl; R2 and R3, together with the atoms to which they are attached, may form a 4-8 membered ring; R5 = alkyl, cycloalkyl, aryl, etc.; L1 = S, SO, SO2, CO, etc.; L2 = a bond, O, S, SO, etc.; W = O, S, (un)substituted NH, N(CN); X = (CH2)naryl, (CH2)nheteroaryl; Y = monocyclic (hetero)aryl; Z = CONH2, CO2R, PO3R, SO3R, etc.; R = H, alkyl, cycloalkyl, etc.; n = 0-2], novel antagonists of α4β1 integrin and/or α4β7 integrin useful in preventing or treating an immune or inflammatory diseases or disorders, were prepared and formulated. Thus, reacting 2-amino-N-cyclohexyl-N-methylbenzamide with (S)-3-[4-(2,6-dichlorobenzoylamino)phenyl]-2-isocyanatopropionic acid Me ester (preparation given) in CH2Cl2 (yield 50%) followed by hydrolysis of the intermediate ester (77%) afforded (S)-II which showed IC50 of < 100 nM in the α4β1 assay.

IT 444086-35-5P 444086-37-7P 444086-39-9P
444086-41-3P 444086-43-5P 444086-52-6P
444086-61-7P 444086-63-9P 444086-65-1P
444086-67-3P 444086-69-5P 444086-71-9P
444086-73-1P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of ureas as integrin alpha 4 antagonists)

RN 444086-35-5 CAPLUS

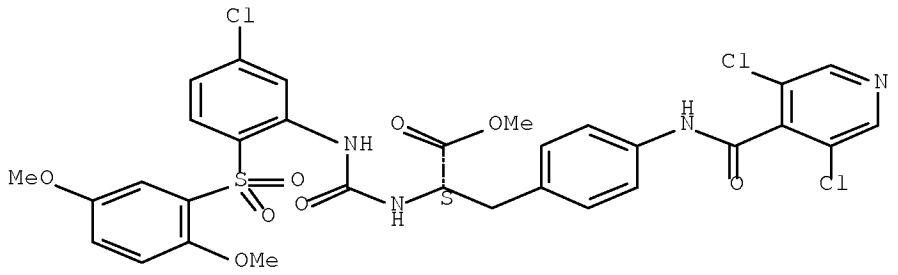
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[[2-(1-piperidinylsulfonyl)phenyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



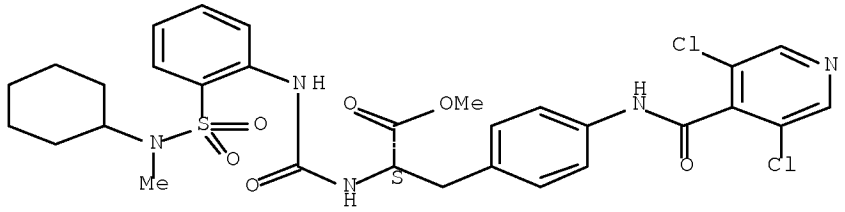
RN 444086-37-7 CAPLUS
CN L-Phenylalanine, N-[[[5-chloro-2-[(2,5-dimethoxyphenyl)sulfonyl]phenyl]amino]carbonyl]-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



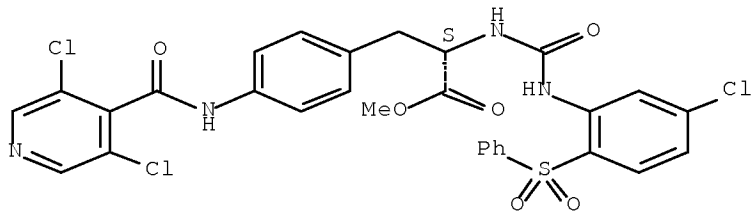
RN 444086-39-9 CAPLUS
CN L-Phenylalanine, N-[[[2-[(cyclohexylmethylamino)sulfonyl]phenyl]amino]carbonyl]-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 444086-41-3 CAPLUS
CN L-Phenylalanine, N-[[[5-chloro-2-(phenylsulfonyl)phenyl]amino]carbonyl]-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, methyl ester (CA INDEX NAME)

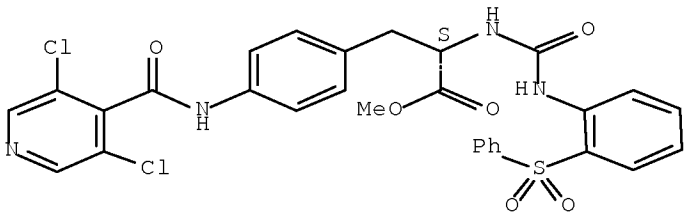
Absolute stereochemistry.



RN 444086-43-5 CAPLUS

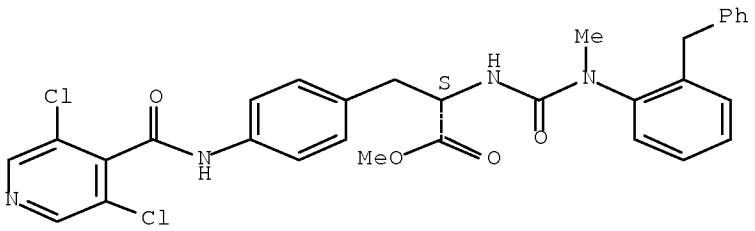
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[[2-(phenylsulfonyl)phenyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



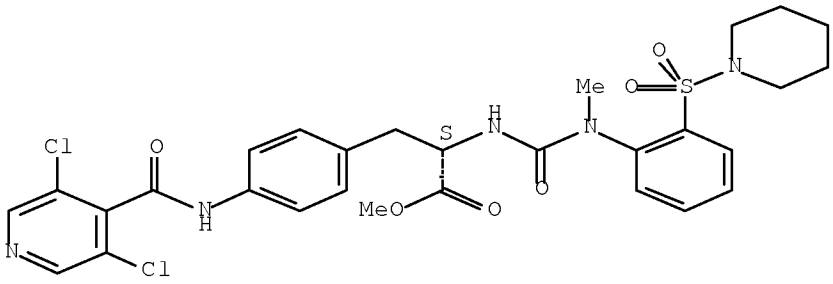
RN 444086-52-6 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[methyl[2-(phenylmethyl)phenyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 444086-61-7 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[methyl[2-(1-piperidinylsulfonyl)phenyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

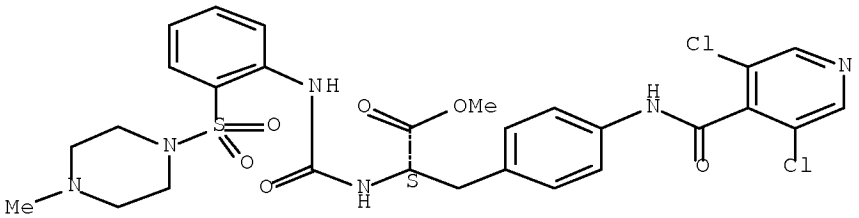
Absolute stereochemistry.



RN 444086-63-9 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[[2-[(4-

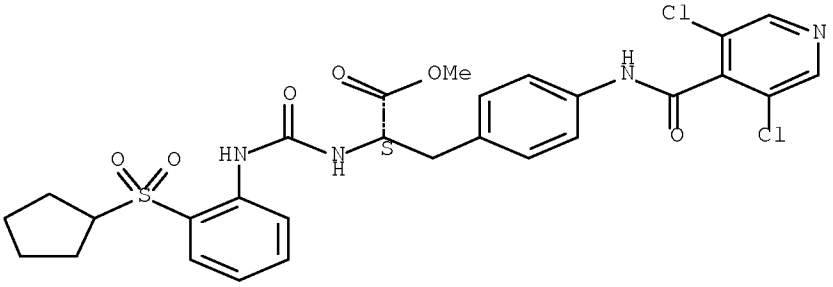
methyl-1-piperazinyl)sulfonyl]phenyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



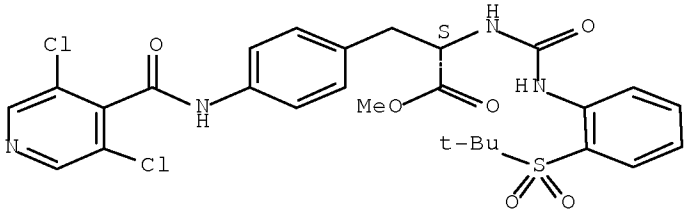
RN 444086-65-1 CAPLUS
CN L-Phenylalanine, N-[[[2-(cyclopentylsulfonyl)phenyl]amino]carbonyl]-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 444086-67-3 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[[2-[(1,1-dimethylethyl)sulfonyl]phenyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

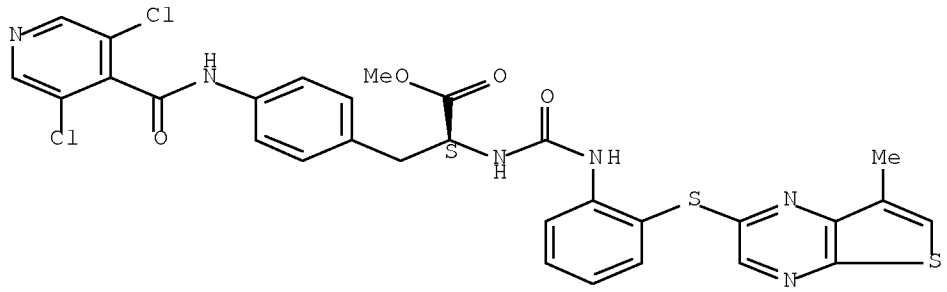
Absolute stereochemistry.



RN 444086-69-5 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[[2-[(7-methylthieno[2,3-b]pyrazin-2-yl)thio]phenyl]amino]carbonyl]-, methyl ester

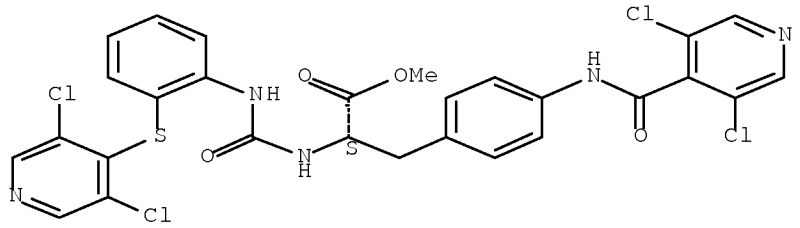
(CA INDEX NAME)

Absolute stereochemistry.



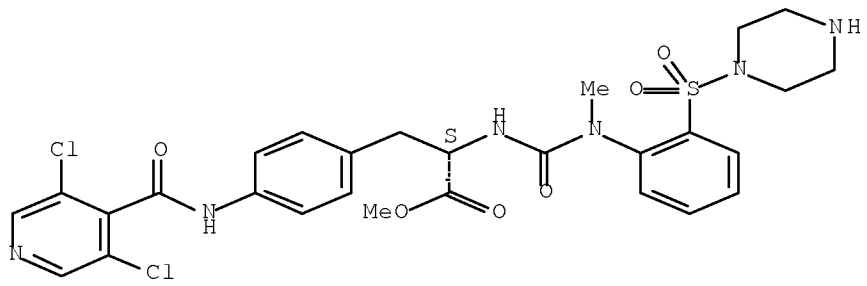
RN 444086-71-9 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[[2-[(3,5-dichloro-4-pyridinyl)thio]phenyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 444086-73-1 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[methyl[2-(1-piperazinylsulfonyl)phenyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

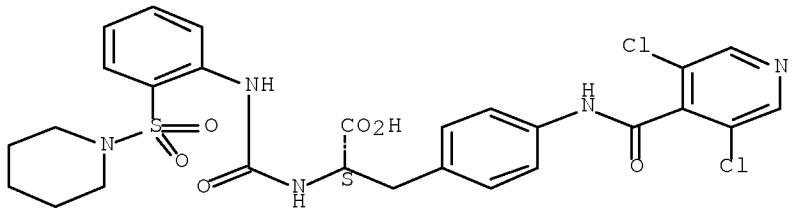
Absolute stereochemistry.



IT 444086-36-6P 444086-38-8P 444086-40-2P
444086-42-4P 444086-44-6P 444086-51-5P
444086-53-7P 444086-54-8P 444086-55-9P
444086-56-0P 444086-57-1P 444086-58-2P
444086-59-3P 444086-60-6P 444086-62-8P
444086-64-0P 444086-66-2P 444086-68-4P
444086-70-8P 444086-72-0P 444086-74-2P
444086-75-3P 444086-76-4P 444086-77-5P
444086-78-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of ureas as integrin alpha 4 antagonists)

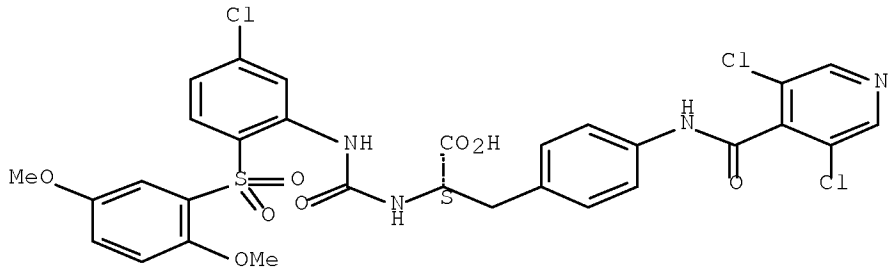
RN 444086-36-6 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[[2-(1-piperidinylsulfonyl)phenyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



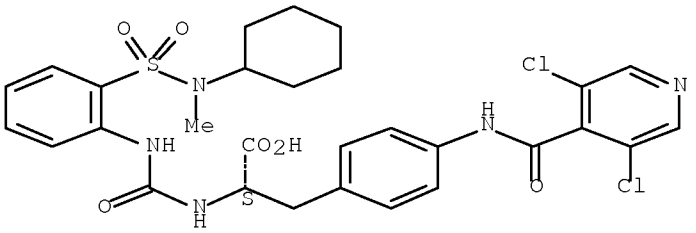
RN 444086-38-8 CAPLUS
CN L-Phenylalanine, N-[[[5-chloro-2-[(2,5-dimethoxyphenyl)sulfonyl]phenyl]amino]carbonyl]-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



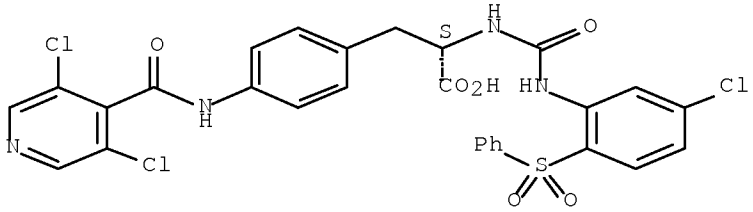
RN 444086-40-2 CAPLUS
CN L-Phenylalanine, N-[[[2-[(cyclohexylmethylamino)sulfonyl]phenyl]amino]carbonyl]-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



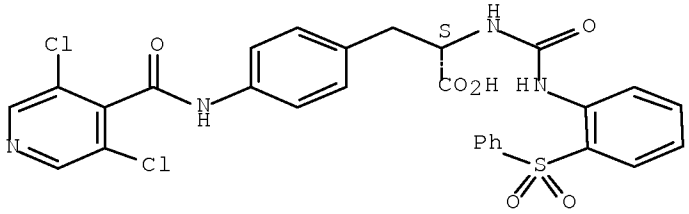
RN 444086-42-4 CAPLUS
CN L-Phenylalanine, N-[[[5-chloro-2-(phenylsulfonyl)phenyl]amino]carbonyl]-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



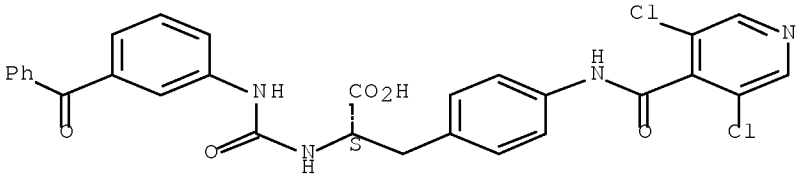
RN 444086-44-6 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[[2-(phenylsulfonyl)phenyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



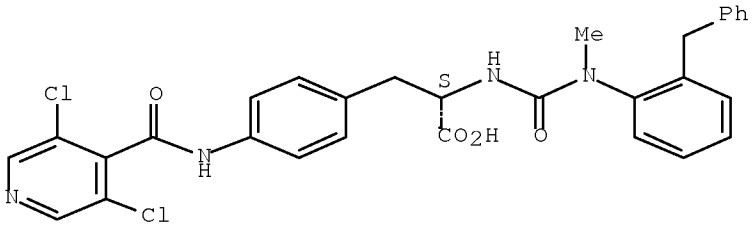
RN 444086-51-5 CAPLUS
CN L-Phenylalanine, N-[[(3-benzoylphenyl)amino]carbonyl]-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



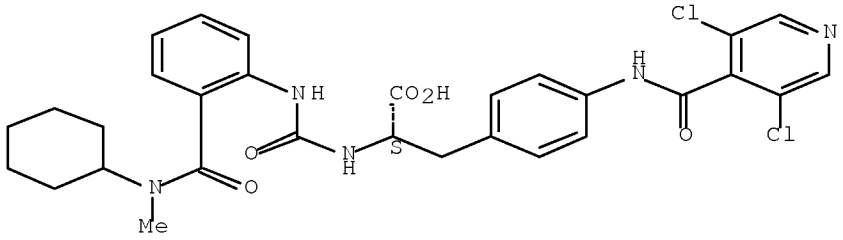
RN 444086-53-7 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[methyl[2-(phenylmethyl)phenyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



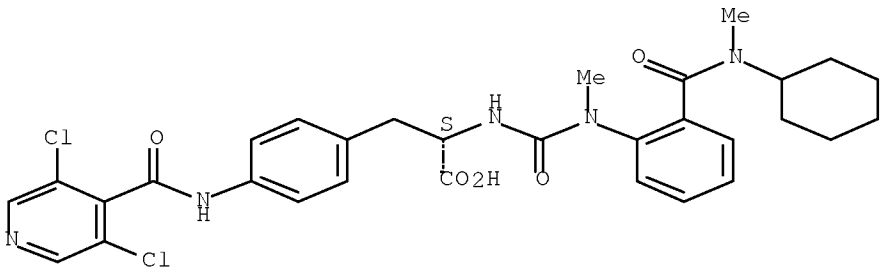
RN 444086-54-8 CAPLUS
CN L-Phenylalanine, N-[[[2-[(cyclohexylmethylamino)carbonyl]phenyl]amino]carbonyl]-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



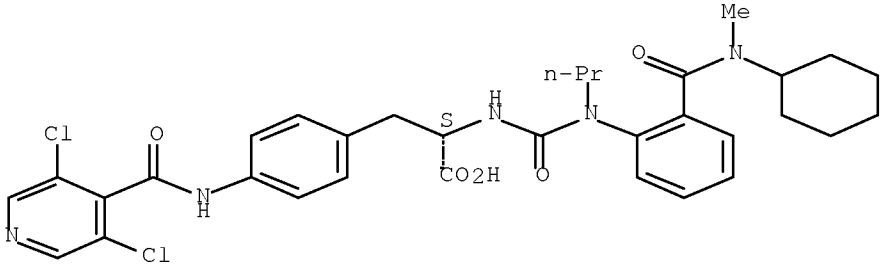
RN 444086-55-9 CAPLUS
CN L-Phenylalanine, N-[[[2-[(cyclohexylmethylamino)carbonyl]phenyl]methylamino]carbonyl]-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



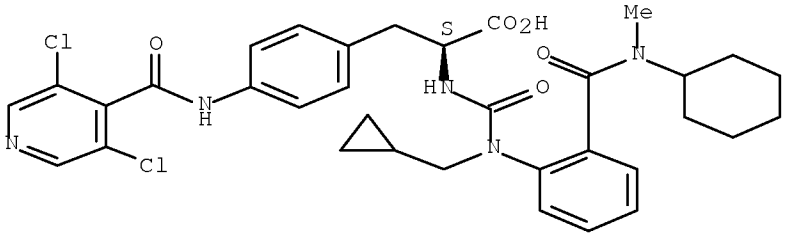
RN 444086-56-0 CAPLUS
CN L-Phenylalanine, N-[[[2-[(cyclohexylmethylamino)carbonyl]phenyl]propylamino]carbonyl]-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



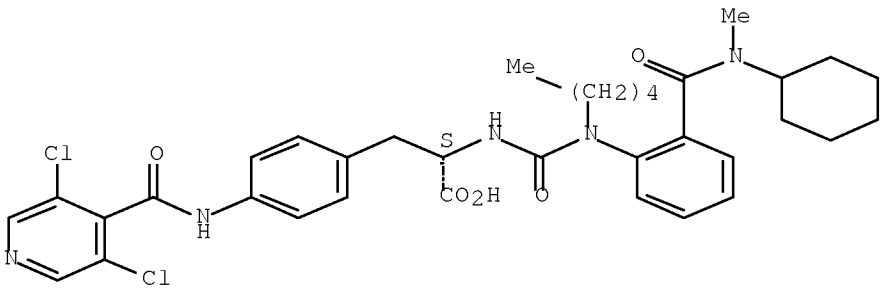
RN 444086-57-1 CAPLUS
CN L-Phenylalanine, N-[[[2-[(cyclohexylmethylamino)carbonyl]phenyl](cyclopropylmethyl)amino]carbonyl]-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



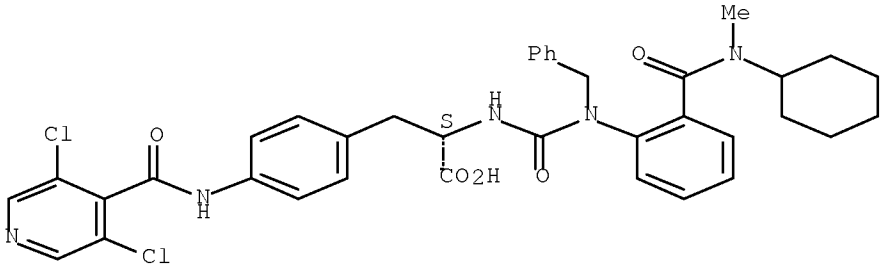
RN 444086-58-2 CAPLUS
CN L-Phenylalanine, N-[[[2-[(cyclohexylmethylamino)carbonyl]phenyl]pentylamino]carbonyl]-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



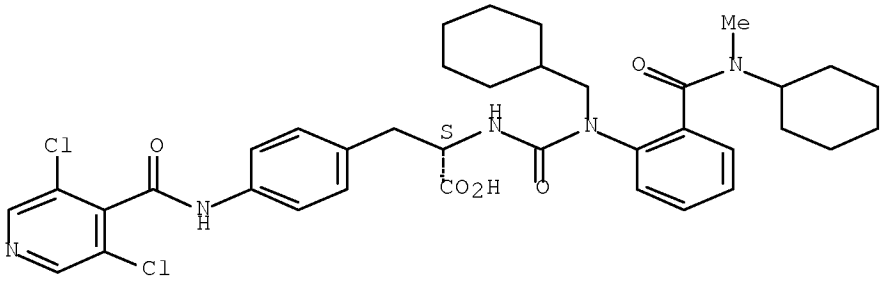
RN 444086-59-3 CAPLUS
CN L-Phenylalanine, N-[[[2-[(cyclohexylmethylamino)carbonyl]phenyl](phenylmethyl)amino]carbonyl]-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



RN 444086-60-6 CAPLUS
CN L-Phenylalanine, N-[[(cyclohexylmethyl)[2-[(cyclohexylmethylamino)carbonyl]phenyl]amino]carbonyl]-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (CA INDEX NAME)

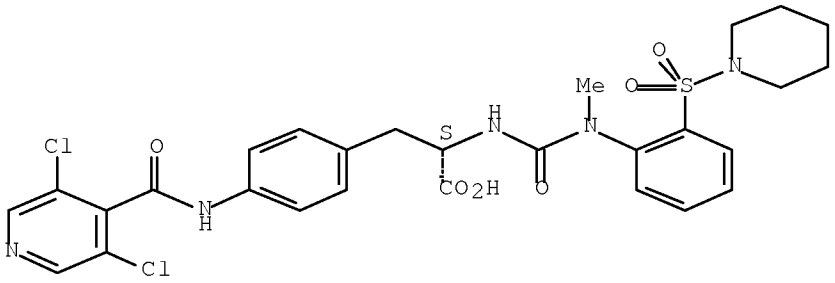
Absolute stereochemistry.



RN 444086-62-8 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-

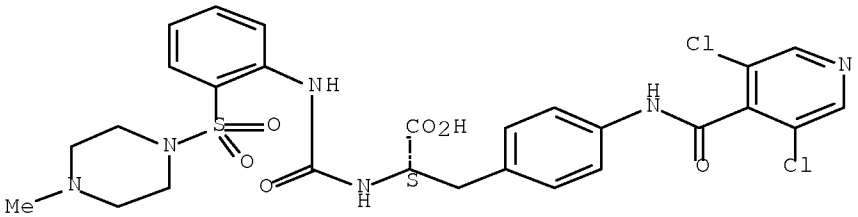
[[methyl[2-(1-piperidinylsulfonyl)phenyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



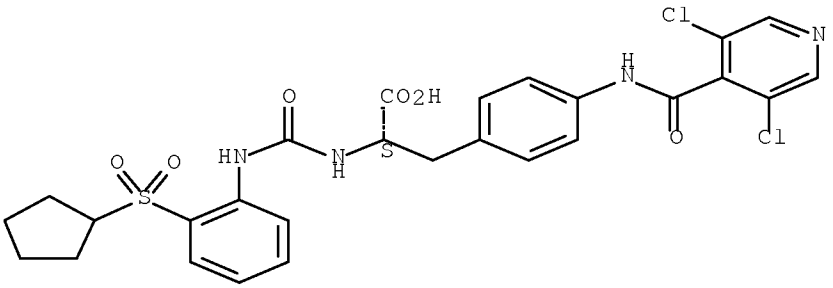
RN 444086-64-0 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[[2-[(4-methyl-1-piperazinyl)sulfonyl]phenyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



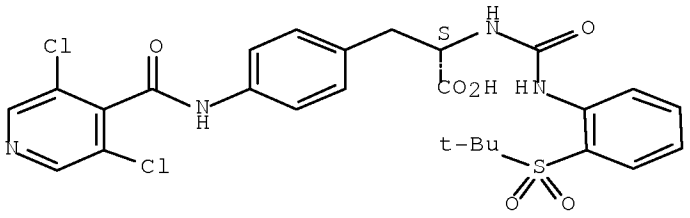
RN 444086-66-2 CAPLUS
CN L-Phenylalanine, N-[[[2-(cyclopentylsulfonyl)phenyl]amino]carbonyl]-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



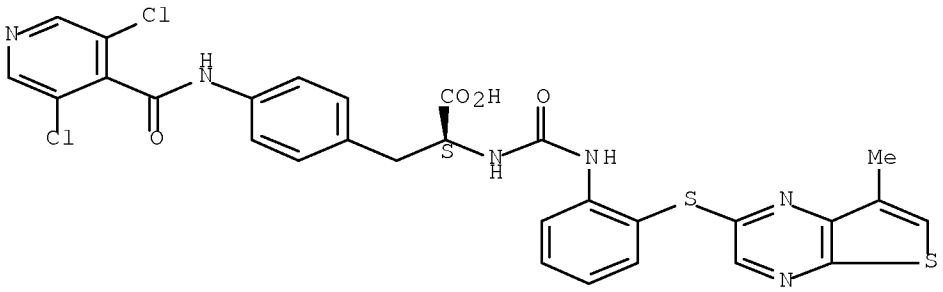
RN 444086-68-4 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[[2-[(1,1-dimethylethyl)sulfonyl]phenyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



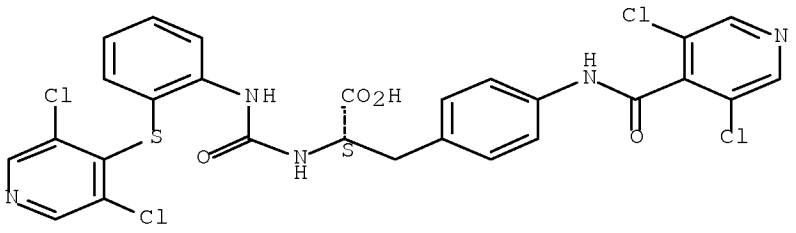
RN 444086-70-8 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[[2-[(7-methylthieno[2,3-b]pyrazin-2-yl)thio]phenyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



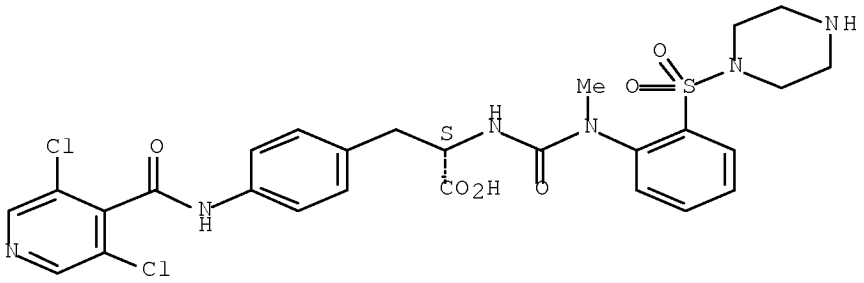
RN 444086-72-0 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[[2-[(3,5-dichloro-4-pyridinyl)thio]phenyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



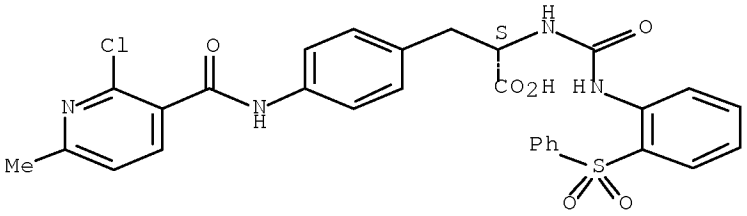
RN 444086-74-2 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[methyl[2-(1-piperazinylsulfonyl)phenyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



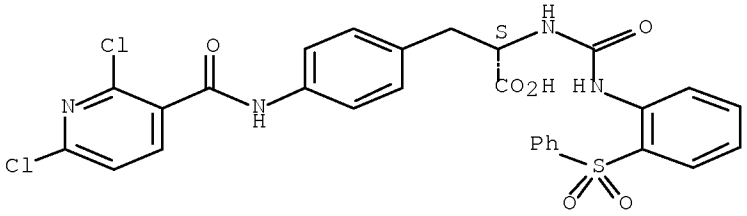
RN 444086-75-3 CAPLUS
CN L-Phenylalanine, 4-[[(2-chloro-6-methyl-3-pyridinyl)carbonyl]amino]-N-[[[2-(phenylsulfonyl)phenyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



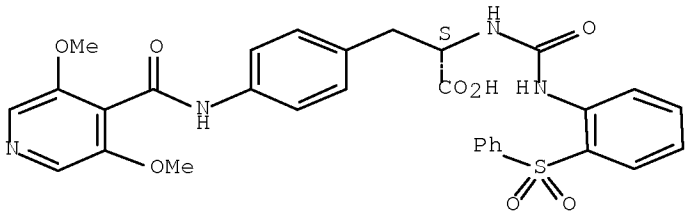
RN 444086-76-4 CAPLUS
CN L-Phenylalanine, 4-[[(2,6-dichloro-3-pyridinyl)carbonyl]amino]-N-[[[2-(phenylsulfonyl)phenyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



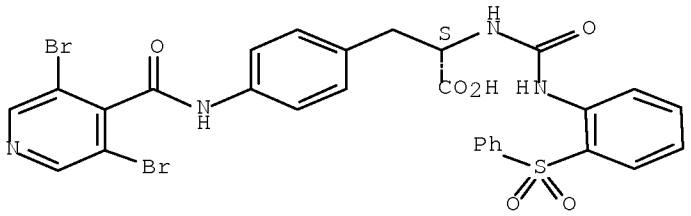
RN 444086-77-5 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dimethoxy-4-pyridinyl)carbonyl]amino]-N-[[[2-(phenylsulfonyl)phenyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



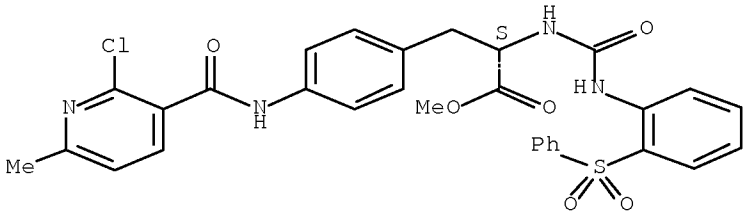
RN 444086-78-6 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dibromo-4-pyridinyl)carbonyl]amino]-N-[[[2-(phenylsulfonyl)phenyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



IT 444087-42-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of ureas as integrin alpha 4 antagonists)
RN 444087-42-7 CAPLUS
CN L-Phenylalanine, 4-[[(2-chloro-6-methyl-3-pyridinyl)carbonyl]amino]-N-[[[2-(phenylsulfonyl)phenyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

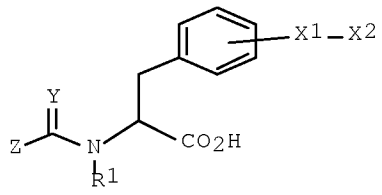


L17 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2002:142667 CAPLUS Full-text
DN 136:200103
TI Preparation of (thio)urea moiety-containing heterocyclic compounds as VLA-4 antagonists
IN Fukui, Hideto; Ikegami, Satoru; Okuyama, Akihiko
PA Kaken Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 43 pp.

CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002014272	A1	20020221	WO 2001-JP6833	20010808
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2001077720	A	20020225	AU 2001-77720	20010808
PRAI JP 2000-241657	A	20000809		
WO 2001-JP6833	W	20010808		

OS MARPAT 136:200103
GI



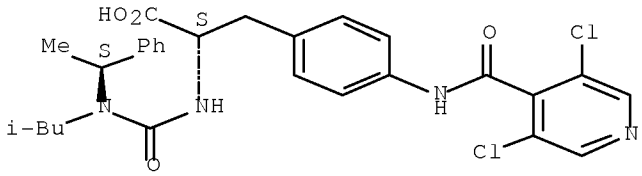
I

AB The title compds. I [R1 = H, alkyl, etc.; X1 = single bond, C.tplbond.C, etc.; Y = O, etc.; Z = NR7R8, etc.; R7, R8 = H, hydrocarbon, etc.; X2 = heterocyclic ring (generic structure given); further details on said heterocyclic ring are given] are prepared A process for the preparation of I is claimed. In an assay for inhibition of VLA-4/VCAM-1 adhesion, 3-[4-[(3,5-dichloropyridine-4-carbonyl)amino]phenyl]-2-(S)-[3-isobutyl-3- [1(S)-phenylethyl]ureido]propionic acid showed IC50 of 1.1 nM.

IT 401470-70-0P 401470-72-2P 401470-73-3P
401470-74-4P 401470-75-5P 401470-84-6P
401470-85-7P 401470-86-8P 401470-87-9P
401470-88-0P 401470-89-1P 401470-90-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (thio)urea moiety-containing heterocyclic compds. as VLA-4 antagonists)

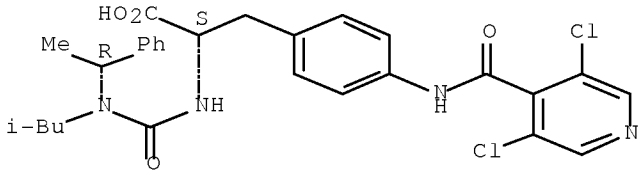
RN 401470-70-0 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[(2-methylpropyl)[(1S)-1-phenylethyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



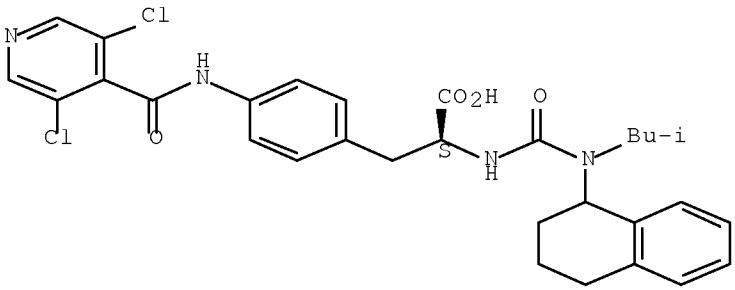
RN 401470-72-2 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[(2-methylpropyl)[(1R)-1-phenylethyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



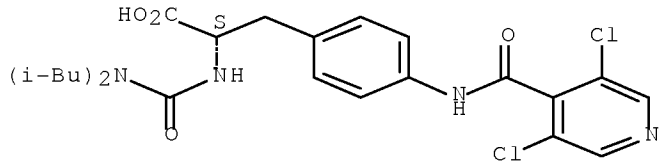
RN 401470-73-3 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[(2-methylpropyl)(1,2,3,4-tetrahydro-1-naphthalenyl)amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



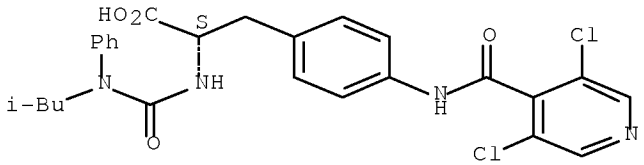
RN 401470-74-4 CAPLUS
CN L-Phenylalanine, N-[[bis(2-methylpropyl)amino]carbonyl]-4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]- (CA INDEX NAME)

Absolute stereochemistry.



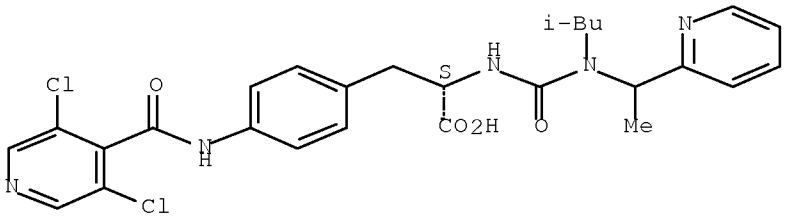
RN 401470-75-5 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[(2-methylpropyl)phenylamino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



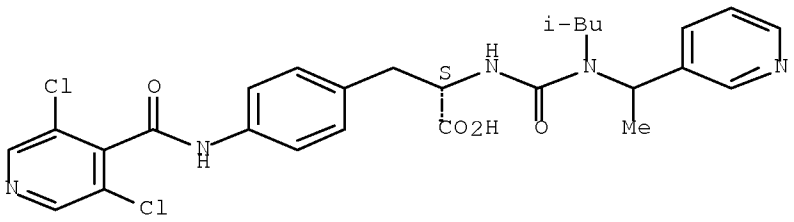
RN 401470-84-6 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[(2-methylpropyl)[1-(2-pyridinyl)ethyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



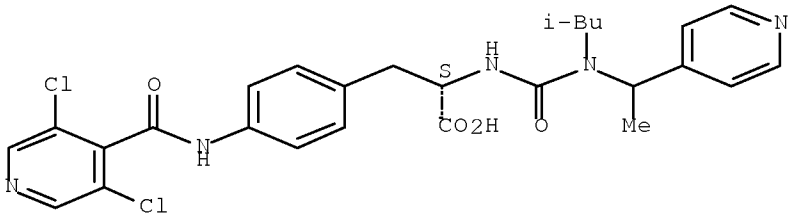
RN 401470-85-7 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[(2-methylpropyl)[1-(3-pyridinyl)ethyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



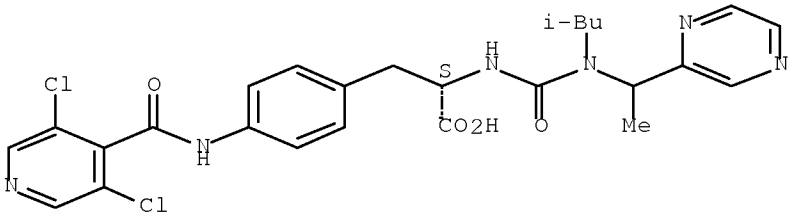
RN 401470-86-8 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[(2-methylpropyl)[1-(4-pyridinyl)ethyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



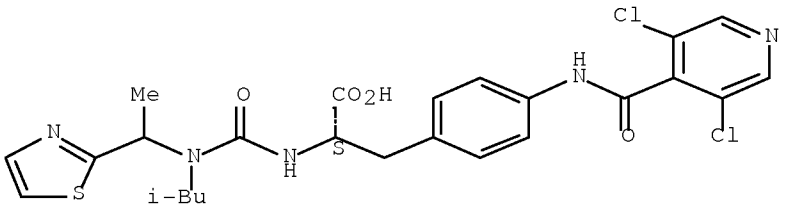
RN 401470-87-9 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[(2-methylpropyl)(1-pyrazinylethyl)amino]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



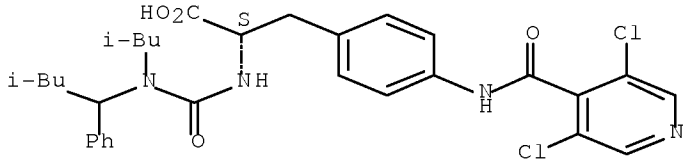
RN 401470-88-0 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[(2-methylpropyl)[1-(2-thiazolyl)ethyl]amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



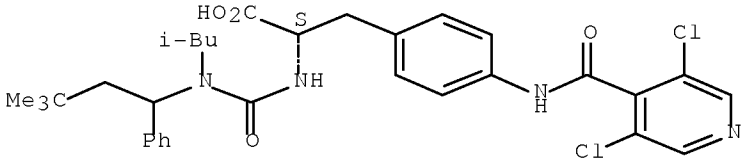
RN 401470-89-1 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[(3-methyl-1-phenylbutyl)(2-methylpropyl)amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



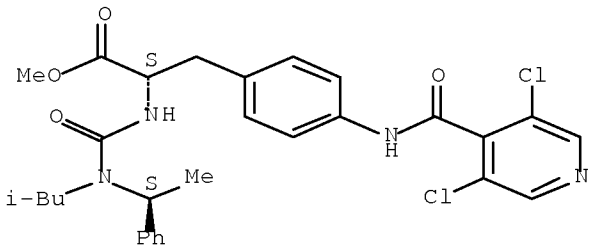
RN 401470-90-4 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[(3,3-dimethyl-1-phenylbutyl)(2-methylpropyl)amino]carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



IT 401471-09-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (thio)urea moiety-containing heterocyclic compds. as VLA-4 antagonists)
RN 401471-09-8 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[[(2-methylpropyl)[(1S)-1-phenylethyl]amino]carbonyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1999:795785 CAPLUS Full-text
DN 132:36028
TI Preparation of phenylalanine derivatives as integrin inhibitors
IN Porter, John Robert; Head, John Clifford; Warrellow, Graham John; Archibald, Sarah Catherine
PA Celltech Therapeutics Limited, UK
SO PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

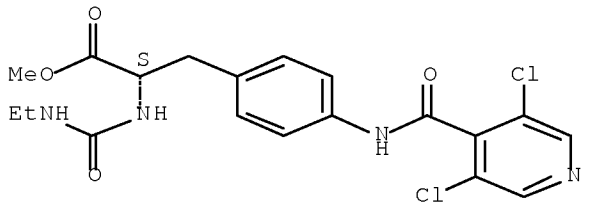
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9964390	A1	19991216	WO 1999-GB1758	19990604
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 9942765	A	19991230	AU 1999-42765	19990604
	EP 1082294	A1	20010314	EP 1999-955469	19990604
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 2002517480	T	20020618	JP 2000-553400	19990604
	US 6911451	B1	20050628	US 1999-326020	19990604
PRAI	GB 1998-12088	A	19980605		
	WO 1999-GB1758	W	19990604		

OS MARPAT 132:36028
AB Phenylalanine derivs. p-[R1(Alk1)r(L1)s]C6H4(Alk2)mCRR2X1R4 [R is a carboxylic acid or derivative; R1 = (un)substituted cycloaliph., polycycloaliph., heterocycloaliph., polyheterocycloaliph., aromatic, or heteroarom. group; Alk1 = (un)substituted aliphatic or heteroaliph. chain; L1 is a linker atom or group; r, s, m = 0 or 1; Alk2 = alkylene; R2 = H, Me; X1 = NR3CO, NR3SO2, NR3CO2, or NR3CONR3a (R3, R3a = H or alkyl); R4 = (un)substituted aliphatic cycloaliph., or polycycloaliph. group] were prepared for use as α4 integrin inhibitors. Thus, N-isobutyryl-N'-(3,5- dichloroisonicotinoyl)-L-4-aminophenylalanine was prepared via acylation/saponification of N'-(3,5-dichloroisonicotinoyl)-L-4-aminophenylalanine Me ester. The compds. of the

invention generally have IC50 values in the α4β1 and α4β7 assays of 1 μM and below.

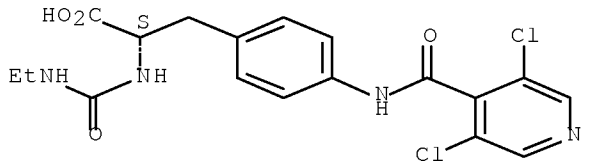
IT 252328-03-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of phenylalanine derivs. as integrin inhibitors)
RN 252328-03-3 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[(ethylamino)carbonyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



IT 252328-04-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phenylalanine derivs. as integrin inhibitors)
RN 252328-04-4 CAPLUS
CN L-Phenylalanine, 4-[[(3,5-dichloro-4-pyridinyl)carbonyl]amino]-N-[(ethylamino)carbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> log hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	22.28	459.09

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-3.20	-5.60

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 16:51:16 ON 11 JUL 2008